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# Stoichiometric analysis of air oxygen consumption in modern vehicles using natural and synthetic fuels

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**Abstract.** The study presents analysis results obtained for stoichiometric reactions of fuel oxidization in air for various motor fuels (such as gasoline, diesel fuel, gaseous fuel) and for biomass-converted and coal-based artificial fuels (such as ethanol, methanol, etc.) and also for hydrogen. Based on the analysis results, comparison is carried out for the specific air consumptions and carbon dioxide emissions of the combustion products.

At a temperature of, which is an ultimate combustion process temperature to be dictated by the achievable properties of structural materials made available for the state-of-the-art engine engineering, the air excess factors are found, the actual air and fuel consumptions are determined, and carbon dioxide emissions are evaluated for the variety of fuels.

The calculated data are presented for the greenhouse effect caused by the use of the various natural and synthetic fuels in transport applications.

In the cases of using hydrocarbon and hydrogen fuels, an abnormally high consumption of the atmospheric air is theoretically evaluated. To reduce the environmental impact, methane-based fuels, bio-ethanol and bio-methanol-based fuels are to be recommended for wider transport vehicle applications.

The analysis method presented in the study offers a universal tool to be instrumental in performing analysis of any fuel compositions both already existing and to be developed for future applications.

**Keywords:** stoichiometry, motor fuels, gasoline, diesel, ethanol, methanol, hydrogen.

## 1. Introduction

The use of any fuel occurs as a result of their huge air flow oxidation with formation of polluting carbon dioxide and water vapor. Known environmental impact studies environment emissions engines operating on refined petroleum products [1]. However, in a world increasingly acquire new fuels derived from plant materials, synthesis gas (methanol), fermentation of glucose (ethanol), the decomposition of water into hydrogen and oxygen (including renewable energy) of natural and anthropogenic hydrocarbons by their conversion [2–6]. These types of fuels for harmful emissions from their air-oxidation on the environment not investigated. In this work, performed a quantitative analysis of the air pollution of the atmosphere carbon dioxide and water vapor for common synthetic fuels. The influence of air flow coefficient on output of harmful emissions. The results are compared with the emissions from the oxidation of fuels derived from petroleum.



## 2. Methods of analysis of the influence of oxidation of fuels pollution Environment

### 2.1. Analysis of the stoichiometric oxidation of fuels when air flow coefficient equal to 1 ( $\alpha = 1$ ).

It is known that complete oxidation of fuel in the air stehiometriceskimi is described by equations that depend on the chemical composition of the fuel. Composition when  $\alpha = 1$  is the theoretical ratio of fuel and air, which in the process of oxidation of oxygen of the air and fuel to be spent completely without residue.

In a general form [7], the stoichiometric equations for hydrocarbon fuels and alcohols are expressed with the Equations (1), (2) as follows:

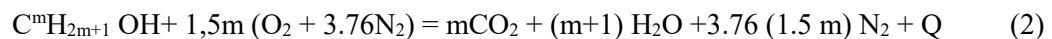
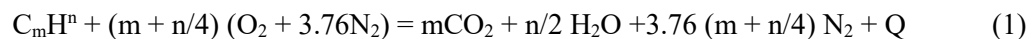


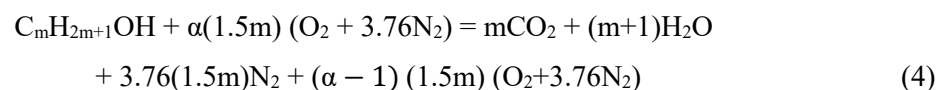
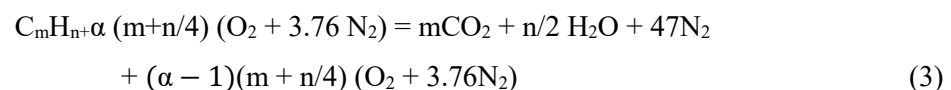
Table 1 summarizes the air to fuel ratio data for the most common types of motor fuels.

**Table 1.** Stoichiometric equation oxidation for common fuels when  $\alpha = 1$ .

Fuel	Formula	Stoichiometric ratio
Hydrogen	H <sub>2</sub>	H <sub>2</sub> +0.5(O <sub>2</sub> +3.76 N <sub>2</sub> )=H <sub>2</sub> O + 1.88N <sub>2</sub>
Ethanol	C <sub>2</sub> H <sub>5</sub> OH	C <sub>2</sub> H <sub>5</sub> OH+3(O <sub>2</sub> +3.76 N <sub>2</sub> )=2CO <sub>2</sub> +3H <sub>2</sub> O + 11.28N <sub>2</sub>
Methanol	C H <sub>3</sub> OH	C H <sub>3</sub> OH+1.5(O <sub>2</sub> +3.76 N <sub>2</sub> )=CO <sub>2</sub> +2H <sub>2</sub> O + 5.64N <sub>2</sub>
Gasoline	C <sub>7</sub> H <sub>16</sub>	C <sub>7</sub> H <sub>16</sub> +11(O <sub>2</sub> +3.76 N <sub>2</sub> )=7CO <sub>2</sub> +8H <sub>2</sub> O + 41.36N <sub>2</sub>
Diesel	C <sub>8</sub> H <sub>18</sub>	C <sub>8</sub> H <sub>18</sub> +12.5(O <sub>2</sub> +3.76 N <sub>2</sub> )=8CO <sub>2</sub> +9H <sub>2</sub> O + 47N <sub>2</sub>
Methane	CH <sub>4</sub>	CH <sub>4</sub> +2(O <sub>2</sub> +3.76N <sub>2</sub> )=CO <sub>2</sub> +2H <sub>2</sub> O+7.52N <sub>2</sub>

### 2.2. Analysis of the stoichiometric oxidation of fuels with an air flow of larger units of $\alpha > 1$ .

However, modern internal combustion engines are designed to operate at much lower combustion temperatures, which is fed into the working volume of the engine fuel mixtures, fortified with excess air. The ratio of the actual flow rate of oxidant (air) to the required for complete oxidation is characterized by excess air coefficient- $\alpha$ . In this case, the formula (1) and (2) acquire the following form:



### 2.3. Analysis of the influence of air flow coefficient on temperature oxidation of fuels ( $\alpha = 1$ ).

According to the stoichiometric equation, oxidation of fuel is characterized with a certain temperature of combustion process described with Equation (5) [8]

$$Q_H^p = C_d^o(t_d^c) \cdot t_d^c, \quad (5)$$

where  $C_d^o(t_d^c)$  is the true isobaric specific heat of oxidation products at oxidation temperature, measured in MJ/(°kg of fuel), and  $t_d^c$  is theoretical oxidation temperature, °C.

The method for determining theoretical oxidation temperature actually means [8, 9] finding a temperature, in the adiabatic conditions, at which the equality of combustion products enthalpies occurs  $C_d^o(t_d^c) \cdot t_d^c$ , and finding the lowest heat of fuel combustion  $Q_H^p$ .

Table 2 summarizes the calculation results, oxidation temperatures, air consumptions and oxidation product yields at  $\alpha = 1$ .

It is seen from Table 2 that at  $\alpha = 1$  complete oxidation of fuel occurs at elevated temperatures, with a large amount of free air being consumed. Fuels that consume especially great volumes of air are hydrogen, gasoline, diesel fuel, and methane.

**Table 2.** Air consumption and oxidation product yields at  $\alpha = 1$

Fuel	Heat of combustion, MJ/kg	Theoretical oxidation temperature, °C	Air consumption, kg/kg of fuel	CO <sub>2</sub> emission, kg/kg of fuel	Specific fuel consumption, kg/MJ	Specific air consumption, kg/MJ	Specific CO <sub>2</sub> emission, kg/Mj	Specific H <sub>2</sub> O yield, kg/MJ
Hydrogen	121	2020	34.32	0	0.0083	0.284	0.000	0.061
Ethanol	27.785	1880	8.95	1.91	0.0360	0.322	0.069	0.152
Methanol	21.131	1900	6.44	1.38	0.0473	0.305	0.065	0.252
Gasoline	44	1850	15.1	3.08	0.0227	0.343	0.070	0.074
Diesel	41.8	1780	15	3.08	0.0239	0.359	0.074	0.082
Methane	49.09	1860	17.16	2.75	0.0204	0.350	0.056	0.093

#### 2.4. Analysis of the influence of air flow coefficient on temperature oxidation of fuels when $\alpha > 1$

In the process of oxidation of the fuel mixture with excess air combustion of the fuel used for heating of the oxidation products (if  $\alpha = 1$ ) and excess air to a temperature of  $t_d$ . Let us consider oxidation at a temperature  $t_d = 1400$  °C, which corresponds to the level of temperatures achievable in the state-of-the-art engine designs [10]. In this case, fuel oxidation reaction takes somewhat different form (Table 3).

**Table 3.** Dependence of excess air ratio of fuel

Fuel	Excess air factor $\alpha$	Formula
Hydrogen	1.7	$H_2 + 0.85(O_2 + 3.76 N_2) = H_2O + 3.196N_2 + 0.35O_2$
Ethanol	1.55	$C_2H_5OH + 4.66(O_2 + 3.76 N_2) = 2CO_2 + 3H_2O + 17.52N_2 + 1.66O_2$
Methanol	1.5	$CH_3OH + 2.25(O_2 + 3.76 N_2) = CO_2 + 2H_2O + 8.46N_2 + 0.75O_2$
Gasoline	1.6	$C_7H_{16} + 17.6(O_2 + 3.76 N_2) = 7CO_2 + 8H_2O + 66.176N_2 + 6.6O_2$
Diesel	1.4	$C_8H_{18} + 17.5(O_2 + 3.76 N_2) = 8CO_2 + 9H_2O + 65.8N_2 + 5O_2$
Methane	1.43	$CH_4 + 2.86(O_2 + 3.76N_2) = CO_2 + 2H_2O + 10.7536N_2 + 0.86O_2$

Heat loss for dissipation into environment and for dissociation of CO<sub>2</sub> and H<sub>2</sub>O and initial fuel and air temperatures are assumed negligible. In this case, Equation (3) takes the form:

$$Q_H^p = [C_d^o(t_d) + (\alpha - 1)C_a^o(t_d)]t_d, \quad (6)$$

where  $C_d^o(t_d)$  is the true specific heat of oxidation products at a temperature of  $t_d$ , kJ/K·kg of fuel,  $C_a^o(t_d)$  is the true isobaric heat of air at a temperature  $t_d$ , kJ/K·kg of fuel,  $Q_H^p$  is the lowest fuel oxidation heat, kJ/kg of fuel,  $\alpha$  is the air excess factor for fuel oxidation; and  $t_d$  is the temperature of oxidation products, °C.

From Equation (6) we find the value of  $\alpha$  factor at the initial temperature of fuel and air as  $t_a = 0$ ,  $t_f = 0$  and the temperature of combustion products  $t_d$  in the form

$$\alpha = 1 + [Q_H^p - C_d^o(t_d)]/[C_a^o(t_d)]. \quad (7)$$

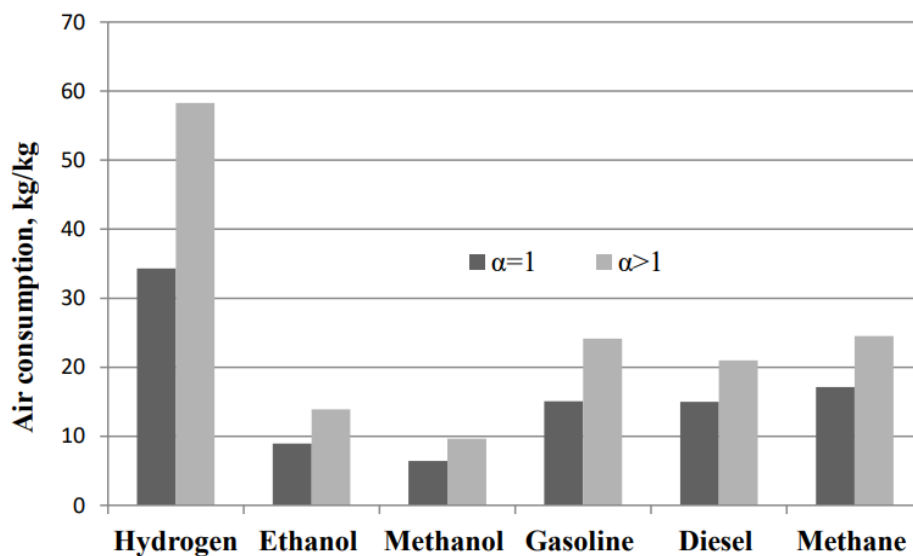
Table 4 summarizes the results of calculating the excess air factor, air consumption and oxidation product yields.

**Table 4.** Excess air factor and air consumption, and product yield at an oxidation temperature of 1,400 °C.

Fuel	Air excess factor $\alpha$	Air consumption kg/kg of fuel	Steam, kg/kg of fuel	CO <sub>2</sub> emission, kg/kg of fuel	Specific fuel consumption, kg/MJ	Specific air consumption, kg/MJ	Specific steam yield, kg/MJ	Specific CO <sub>2</sub> emission, kg/MJ
Hydrogen	1.7	58.3	9	0	0.0083	0.482	0.074	0.000
Ethanol	1.55	13.9	1.17	1.91	0.0360	0.500	0.042	0.069
Methanol	1.5	9.65	1.125	1.375	0.0473	0.457	0.053	0.065
Gasoline	1.6	24.16	1.44	3.08	0.0227	0.549	0.033	0.070
Diesel	1.4	21	1.42	3.09	0.0239	0.502	0.034	0.074
Methane	1.43	24.53	2.25	2.75	0.0204	0.500	0.046	0.056

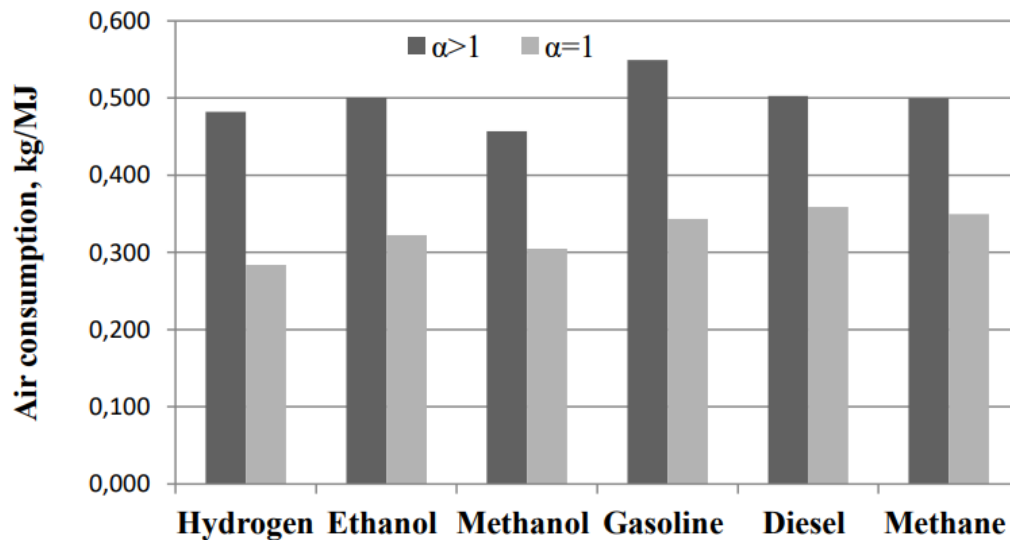
### 3. The results of the study

Analysis of the calculation results demonstrates that there is a considerable difference in the environmental impact caused by various fuels used for a combustion engine. Figures 1–4 display absolute and specific characteristics of fuels such as air consumption, carbon dioxide emissions and steam generation at  $\alpha = 1$  and  $\alpha > 1$ .



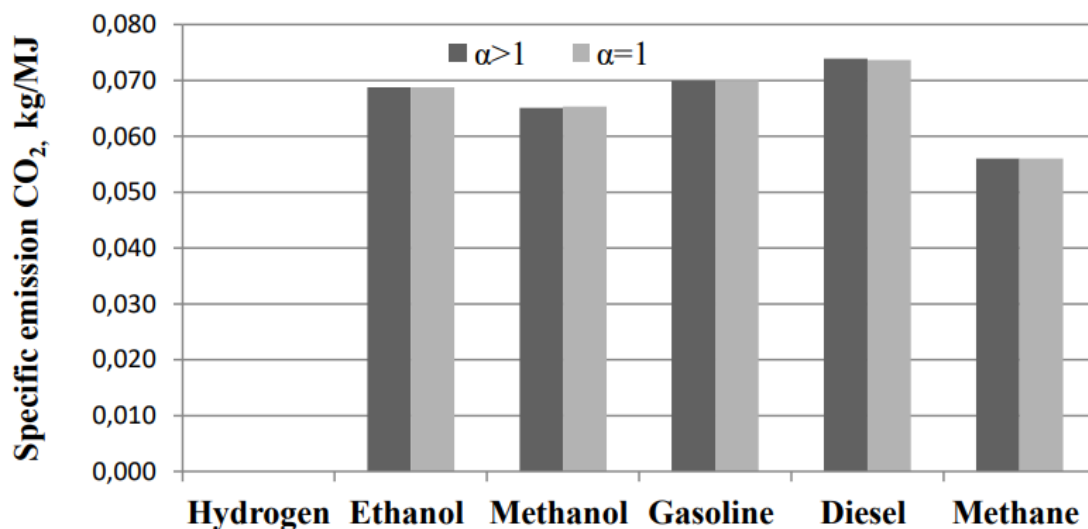
**Figure 1.** Free air consumption

It can be seen from Fig. 1 that the absolute free air consumption is the highest for hydrogen and hydrocarbon types of fuels. Combustion at  $\alpha > 1$  leads to an increase in air combustion for all types of fuel.



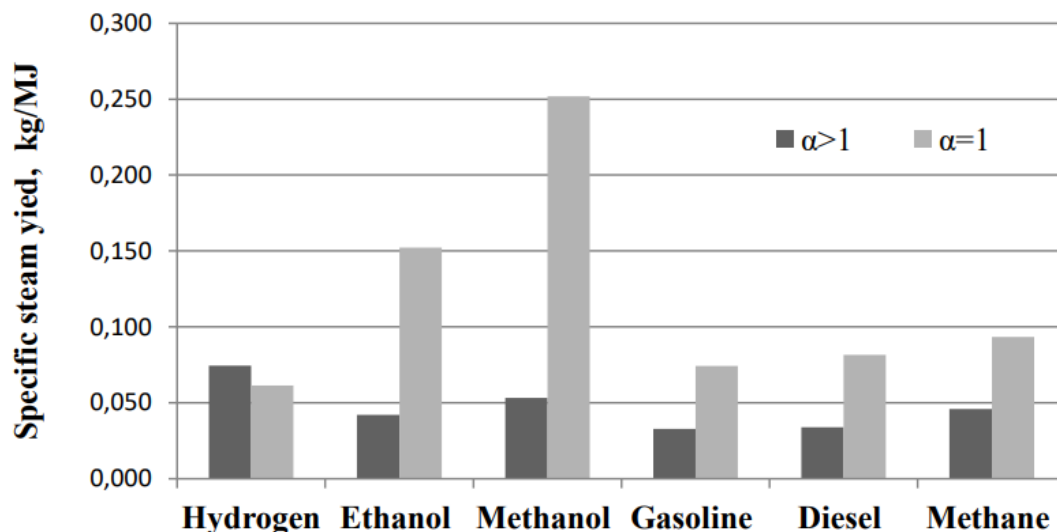
**Figure 2.** Specific free air consumption

However, the difference in the combustion heat (Table 2) leads to the free air consumptions being similar in order to produce similar amounts of energy. The least air consumption is observed for methanol, hydrogen and ethanol. The greatest air consumption is observed for the cases of using gasoline, diesel fuel and methane.



**Figure 3.** Specific CO<sub>2</sub> emission

Carbon dioxide emission is the same for  $\alpha = 1$  and  $\alpha > 1$ , both for hydrocarbon fuels and for alcohols. There is no CO<sub>2</sub> emission for hydrogen oxidation; small values of carbon dioxide emissions are observed for methane and methanol; and the highest emissions are observed for diesel fuel and gasoline.



**Figure 4.** Specific steam yield

Steam is generated most intensely at  $\alpha = 1$ . At  $\alpha > 1$ , the least amount of steam is generated by hydrocarbon fuel and alcohols; and the greatest steam yield is observed for hydrogen fuel.

#### 4. Conclusion

1. The analysis showed that, in an effort to raise the temperature of oxidation of all fuels to the limits defined by the stoichiometric ratio  $\alpha = 1$ , decreased absolute and specific air consumption increases engine efficiency and reduced fuel consumption for 1 kWh of energy.
2. Actual capacities offered by the state-of-the-art engine engineering are limited with the durability characteristics of structural materials and require increased air consumption.
3. The highest carbon dioxide emission occurs in the case of using the most common fuels, such as diesel fuel and gasoline; and the lowest carbon dioxide emission is observed for hydrogen and alcohol-based synthetic fuels.
4. In terms of reducing greenhouse effect and increasing thermodynamic efficiency of engines, most promising appears development of high-temperature combustion engines operating on hydrogen fuel.
5. For state-of-the-art combustion engine designs, a positive environmental effect can be achieved through the use of hydrogen and alcohol-containing fuel compositions and methane-based gaseous fuels.

#### Acknowledgments

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#### References

- [1] Kulchitsky A R 2010 *Toxicity reciprocating internal combustion engine. The formation of harmful substances during combustion of fuels* (Vladimir: Vladimir State University Press)
- [2] Nadir Yilmaz 2017 Sustainable alternative fuels in aviation *Energy* **140** (2) 1378–86
- [3] Yu Bicer and I Dincer 2018 Life cycle environmental impact assessments and comparisons of alternative fuels for clean vehicles *Resources, Conservation and Recycling* **132** 141–57
- [4] Shcheklein S E and Dubinin A M 2018 Production of liquid fuels based on co-current gas generator and nuclear reactor *Atomic energy* **124** (2) 76–9
- [5] Romanova E D, Romanov I D, Vasilyev V A and Chernyshov E A 2011 The development of technology to produce synthetic and life alternatives fuels *Alt. energy and ecology* **6** 81–3

- [6] Veziroglu T N and Sahin S 2014 21-century Energy: hydrogen power *Alt. energy and ecology* **2 (142)** 12–28
- [7] Baehr H B 1988 *Thermodynamik* (Berlin/Heidelberg: Springer-Verlag)
- [8] Lewis B 1968 *Flame Burning. Explosions in gases* (Moscow: Mir)
- [9] Stromberg A G and Semchenko D G 2001 *Physical chemistry* (Moscow: Vysshaya Shkola)
- [10] 1982 *Environmental chemistry* (Moscow: Chemistry)